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COUPLED GEOMECHANICAL SIMULATIONS OF UCG CAVITY EVOLUTION

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Abstract

This paper presents recent work from an ongoing project to develop predictive tools for cavity/combustion-zone growth and to gain quantitative understanding of the processes and conditions (both natural and engineered) affecting underground coal gasification (UCG). In this paper we will focus upon the development of coupled geomechanical capabilities for simulating the evolution of the UCG cavity using discrete element methodologies.

The Discrete Element Method (DEM) has unique advantages for facilitating the prediction of the mechanical response of fractured rock masses, such as cleated coal seams. In contrast with continuum approaches, the interfaces within the coal can be explicitly included and combinations of both elastic and plastic anisotropic response are simulated directly. Additionally, the DEM facilitates estimation of changes in hydraulic properties by providing estimates of changes in cleat aperture.

Simulation of cavity evolution involves a range of coupled processes and the mechanical response of the host coal and adjoining rockmass plays a role in every stage of UCG operations. For example, cavity collapse during the burn has significant effect upon the rate of the burn itself. In the vicinity of the cavity, collapse and fracturing may result in enhanced hydraulic conductivity of the rock matrix in the coal and caprock above the burn chamber. Even far from the cavity, stresses due to subsidence may be sufficient to induce new fractures linking previously isolated aquifers. These mechanical processes are key in understanding the risk of unacceptable subsidence and the potential for groundwater contamination. These mechanical processes are inherently non-linear, involving significant inelastic response, especially in the region closest to the cavity. In addition, the response of the rock mass involves both continuum and discrete mechanical behavior.

We have recently coupled the LDEC (Livermore Distinct Element Code) and NUFT (Non-isothermal Unsaturated Flow and Transport) codes to investigate the interaction between combustion, water influx and mechanical response. The modifications to NUFT are described in detail in a companion paper. This paper considers the extension of the LDEC code and the application of the coupled tool to the simulation of cavity growth and collapse. The distinct element technology incorporated into LDEC is ideally suited to simulation of the progressive failure of the cleated coal mass by permitting the simulation of individual planes of weakness. We will present details of the coupling approach and then demonstrate the capability through simulation of several test cases.

1. Introduction

UCG converts in situ coal into a synthesis gas through the same chemical reactions that occur in surface gasifiers. While the economics of UCG appear to be promising, progress in UCG deployment has been hampered by insufficient modeling methodology and quantitative physical-process understanding. Over the past two decades we have advanced our simulation capabilities and understanding of thermo-hydro-chemical-mechanical (THCM) processes that are of use to UCG and related environmental issues. This paper discusses an ongoing project at LLNL that leverages such advances to develop a simulation capability and a comprehensive quantitative understanding of the UCG-relevant processes. A benefit of this work is to understand how UCG can be engineered to reduce environmental risk, while improving productivity.

The UCG combustion zone will occur in and around a cavity that will be partially filled with caved coal rubble (and possibly caprock rubble) from the roof of the cavity (Figure 1). This zone will propagate between injection and production wells. The rate of cavity/combustion-zone growth depends on a number of factors, some of which can be controlled, such as the rate of air and/or air/steam injection, as well as many natural-system factors, affected by the THCM properties of the coal and surrounding host rock. Host-coal/rock thermal conductivity affects heat conduction. Coal chemistry affects combustion. Permeability (particularly within fracture networks), along with hydrostatic pressure, affects water influx into the combustion zone, the flow of injected and product gas from the cavity into the host coal/rock, the flow of pyrolysis gas, and convective heat transfer in the host coal/rock. Permeability also affects natural convection that can transport aqueous-phase liquids (and contaminants) from the cavity. The ratio of fracture surface area to bulk rock volume affects the potential reaction surfaces for combustion. Geomechanical properties of the fractures and coal/rock matrix affect the stability and caving of roof materials. Fracture properties will dynamically change as combustion proceeds. All of these effects will interact in a highly dynamic, non-linear manner, influencing the growth of the coal cavity within a heterogeneous host-coal/rock environment.

UCG pilot studies have shown the importance of operating within a critical range of injection pressure (the “sweet spot”), which is high enough to keep too much water from invading the combustion zone and quenching the burn, and low enough to minimize loss of product gas and spreading of contaminants from the reactor zone to nearby aquifers. Determining the “sweet spot”, which is scale dependent (pilot versus industrial scale), is crucial for successful UCG operations. A major objective of this proposal is to develop the ability to determine the “sweet spot” for UCG operations.

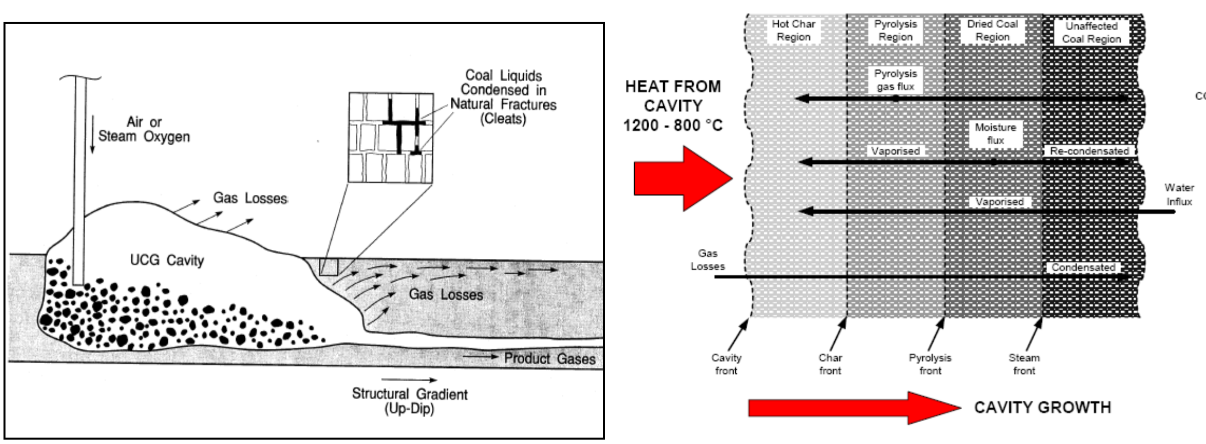

Figure 1: Schematic of the UCG cavity growth process and cavity side walls. Panel (a) is obtained from Covell and Thomas (1996). Panel (b) is from www.berr.gov.uk (2008).

At LLNL we are developing a simulation capability for predicting cavity/combustion-zone growth and for developing a comprehensive quantitative understanding of the processes and conditions (both natural and engineered) affecting underground coal gasification (UCG).

2. Methodology

In order to simulate cavity/combustion-zone growth and develop a quantitative understanding of subsurface THCM processes and conditions affecting UCG, we are enhancing and combining the capabilities of several codes previously developed at LLNL:

NUFT (Nonisothermal Unsaturated-saturated Flow and Transport) is a massively-parallel code used to simulate multiphase, multi-component heat and mass flow and reactive transport in unsaturated and saturated porous media (Nitao, 1998). It has been used to solve complex problems in nuclear waste management (Buscheck et al. 2002, 2003a, 2003b), environmental remediation (e.g., steam-enhanced extraction), and CO2 sequestration. In addition to simulating cavity/combustion-zone growth, NUFT will be used to simulate the transport of injected and product gas into the surrounding hydrogeologic environment. NUFT can also be used to simulate the transport and fate of contaminants generated by the coal-combustion process, as well as CO2 sequestration in the coal cavity after UCG operations have been completed.

LDEC (Livermore Distinct Element Method) is a massively parallel code originally developed to predict the collapse of underground cavities. The current version predicts rock mass failure due to relative motion along pre-existing joints and fracture of initially intact blocks of rock. This is achieved by using a combination of Finite Element and Distinct Element methodologies (Morris et al. 2003, 2006). LDEC is now coupled with fracture network flow and transport solvers to predict the permeability of fracture networks under evolving stress fields (Johnson and Morris, 2009). LDEC is being utilized to predict the stress on the coal cleats in order to investigate the evolving permeability of the coal mass cleat network. In addition, LDEC will provide predictions of cavity collapse.

Thermal-hydrological-chemical conditions in the coal seam and adjoining hydrogeologic units will be calculated using the NUFT code. The NUFT results will then be utilized by the LDEC code, which will determine the impact of those conditions (perturbations to pore pressure and temperature, as well as the consumption of the coal by virtue of combustion) on the geomechanical state of stress, which will alter the permeability of the coal cleat networks and fracture networks in the adjoining caprock and bedrock units, and will also affect the stability of the cavity roof, resulting in failure of the coal and (possibly) the overlying caprock. LDEC-calculated perturbations will then be utilized by the NUFT code. This iterative computational process will continue until a converged solution is obtained.

At this point, the initial phase of the project in underway and an interface is being developed for exchanging results between NUFT and LDEC, but coupled NUFT-LDEC simulations are yet to be executed. In this paper, we present results from LDEC simulations investigating the stability of growing cavities within a coal mass. This initial stage is permitting identification of the most important parametric dependencies between the evolving geomechanical processes and the thermal-hydrological-chemical processes.

3. Geomechanical Simulations of UCG Cavity Evolution using the Livermore Distinct Element Code (LDEC)

The distinct element method (DEM) is a numerical method where the computational domain is treated by distinct solid objects including detailed treatment of the interfaces between the discrete objects. The DEM has been applied to a wide range of problems in geomechanics (see Cundall, 2001 for a review). The Livermore Distinct Element Code (LDEC) implements DEM and Finite Element capabilities for solid response and Smooth Particle Hydrodynamics and Discrete Fracture Network capabilities for fluid response (see Morris and Johnson 2009). Polyhedral block implementations of the DEM are naturally suited to simulating cleated coal structures and heavily jointed rock because the DEM can explicitly accommodate the blocky nature of natural rock masses (see Figure 2).

In this paper, we utilize the LDEC capabilities for simulating deformation of regions containing large numbers of interfaces. Within the intact material, LDEC has several options for treating deformation. The simplest and most computationally efficient is to treat the intact blocks as rigid and assume all compliance occurs at the interfaces. The second level of fidelity in LDEC supports a uniform deformation tensor within each block using the theory of a Cosserat point (Morris et al., 2004). The highest level of fidelity for deformation within the blocks provided by LDEC is to sub-discretize them into finite element blocks. In this study, for simplicity, the rigid block approach is used an all compliance of the coal mass is accommodated by the cleats.

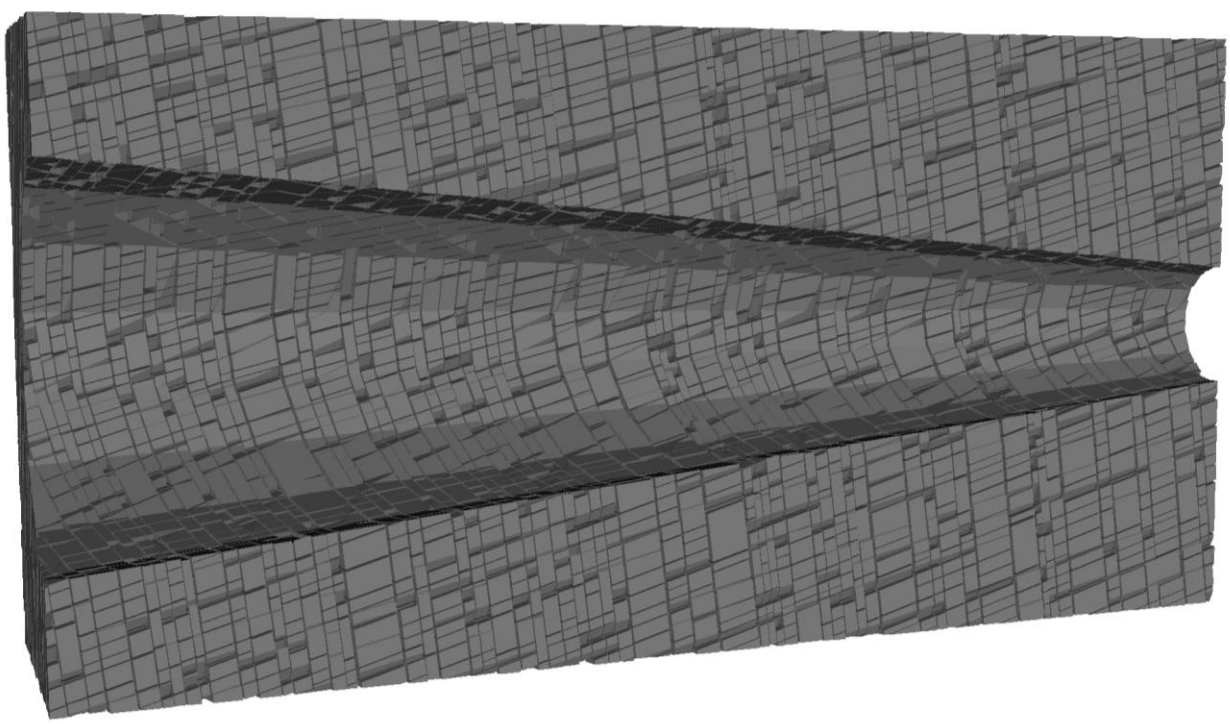

Figure 2: The polyhedral block capability of LDEC allows complicated combinations of cleat and cavity structures.

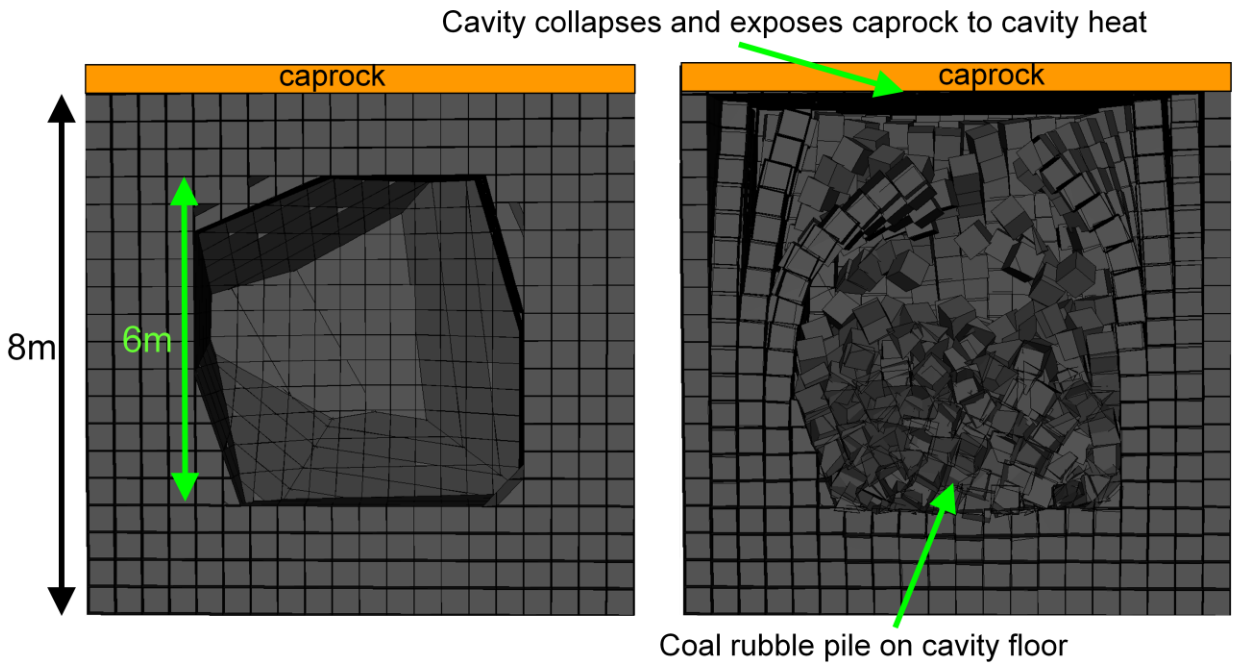

Figure 3: LDEC simulation of cavity collapse in 3-D. This simulation corresponds to the volume of coal consumed by day 3 of the Hoe Creek pilot test.

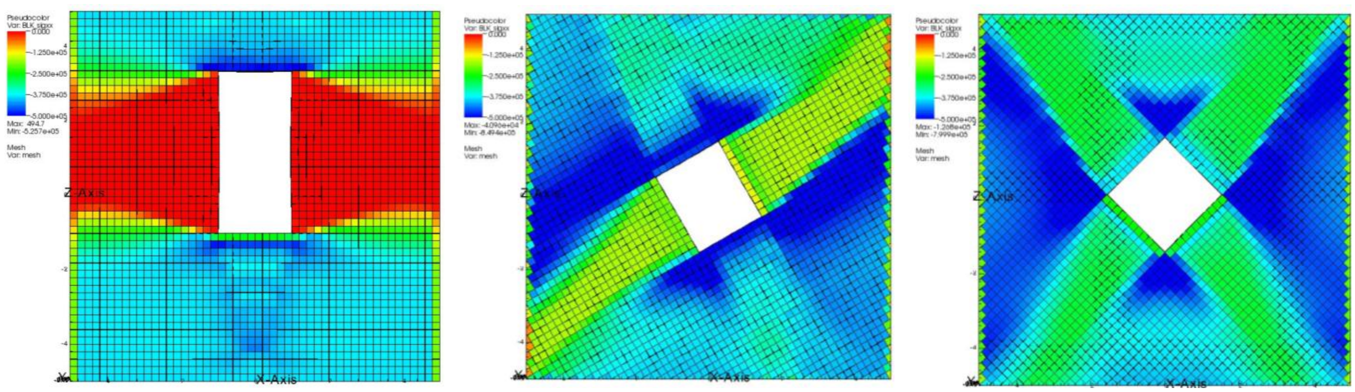

Figure 4: Cavity evolution due to mechanical processes with variable cleat orientation (0, 30 and 45 degrees) from the horizontal. These simulations were performed by assuming an initial, instantaneous cavity and then predicting and removing the portions of the coal mass rendered unstable by the excavation, in the presence of gravity and an insitu stress field.

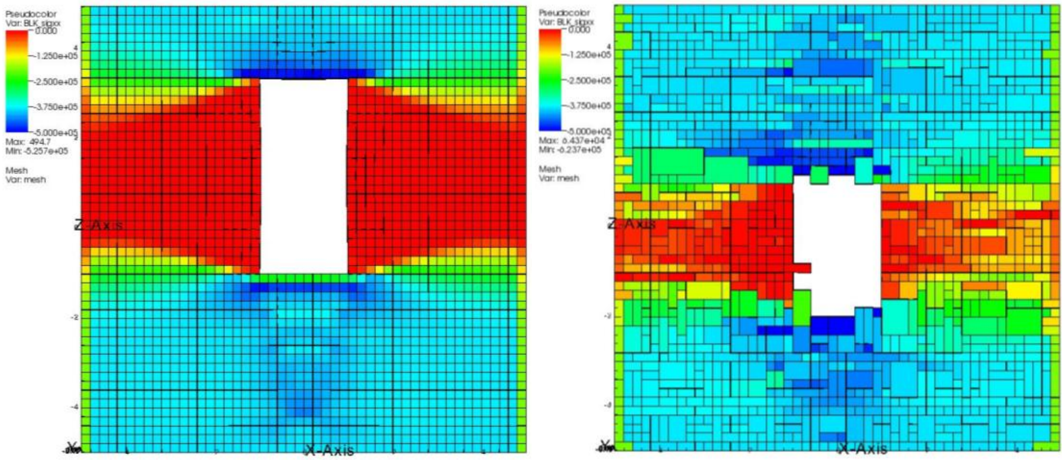

Figure 5: Cavity evolution due to mechanical processes with variable cleat persistence. Specifically, fully persistent cleats (at left) result in a more extensive chimney of failure, while non-persistent cleating results in more oddly shaped coal blocks that lock and arrest the upward propagation of the failure coal mass.

Figure 3 shows an LDEC simulation that demonstrates the versatility of the DEM and highlights the advantages of such an approach for simulating coal cavity collapse. This simulation investigates the stability of a coal bed in response to an evolving burn cavity. It is observed that once the cavity extends to a diameter of 6 m, the roof collapses up to the adjacent caprock. This particular simulation included the detail of rubble accumulation on the flow of the cavity.

Figures 4 and 5 show the lateral stress in the coal mass adjacent to a cavity at a shallow depth of 40m. These simulations were performed by assuming an initial, instantaneous cavity and then predicting and removing the portions of the coal mass rendered unstable by the excavation, in the presence of gravity and an insitu stress field. Consequently, these results show the evolving shape of the stable coal mass in response to mechanical effects alone, and do not include the cavity evolution due to the burn. Once this capability is back coupled with NUFT, the evolution of the cavity due to the burn will also be included. Figure 4 shows an LDEC parameter study of the influence of cleat orientation upon cavity evolution, while Figure 5 demonstrates that cleat persistence also plays a role in controlling the mechanical evolution of the cavity.

4. Summary

We have demonstrated the geomechanical component of an ongoing effort to develop a UCG simulation tool. The results of the parameter identification/sensitivity study once completed will be utilized in the next phase of the project to determine how to best implement the coupled physical processes in the NUFT-LDEC simulation tool. The final stage of this project will involve applying this simulation capability to specific UCG sites, helping guide the site characterization and pilot-scale UCG monitoring, as well as validating the NUFT-LDEC models of those UCG operations.

Once complete, the UCG simulation capability will lead to improved understanding of the complex thermal-hydrological-chemical-mechanical (THCM) processes, natural conditions, and engineering options influencing the growth of the cavity/combustion zone within a coal seam during UCG operations. The knowledge gained will be valuable in guiding site characterization, establishing parameter calibration and model validation strategies that could be implemented in laboratory studies, field testing, and monitoring/history-matching studies of UCG prospects. It will also be applicable to real-time process control in UCG operation and provide valuable insight into how UCG operations can be optimized with respect to productivity and environmental impact.

5. Disclaimer

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6. References

Buscheck, T.A., N.D. Rosenberg, J. Gansemer, and Y. Sun, Thermohydrologic Behavior at an Underground Nuclear Waste Repository at Yucca Mountain, NV, Water Resources Research. 38 (3), 10, 2002.

Buscheck, T.A., N.D. Rosenberg, J.A. Blink, Y. Sun, and J. Gansemer. "Analysis of Thermohydrologic Behavior for Above-Boiling and Below-Boiling Thermal Operating Modes for a Repository at Yucca Mountain," Journal of Contaminant Hydrology, 62-63, 441-457. New York, New York: Elsevier. 2003a.

Buscheck, T.A., L.G. Glascoe K.H. Lee, J. Gansemer, Y. Sun, and K, Mansoor, Validation of the Multiscale Thermohydrologic Model Used for Analysis of a Proposed Repository at Yucca Mountain, Journal of Contaminant Hydrology, 62-63, 421-440, 2003b.

Covell, J. R. and Thomas, M. H., 1996, Combined Air Sparging and Bioremediation of an Underground Coal Gasification Site. EG&G Report DE-AC21-95MC31346.

Cundall, P. A. (2001), A discontinuous future for numerical modeling in geomechanics?, Proc. Inst. Civ. Eng-Geotech. Eng., 149, 41-47.

Johnson, S.M. and J.P. Morris, "Hydraulic fracturing mechanisms in carbon sequestration applications," Proceedings of the American Rock Mechanics Association Meeting, Ashville, 2009.

Morris, J. P. and S. M. Johnson (2009) "Dynamic simulations of geological materials using combined FEM/DEM/SPH analysis", Geomechanics and Geoengineering, 4:1,91-101

Morris, J.P., M.B. Rubin, S.C. Blair, L.A. Glenn, F.E. Heuze, "Simulations of Underground Structures Subjected to Dynamic Loading using the Distinct Element Method", Engineering Computations, Vol. 21 (2/3/4), 384-408. 2003.

Morris, J.P., M.B. Rubin, G.I. Block and B.P. Bonner, "Simulations of fracture and fragmentation of geologic materials using combined FEM/DEM analysis", International Journal of Impact Engineering, 33, 463-473. 2006.

Nitao, J.J, "Reference Manual for the NUFT Flow and Transport Code, Version 2.0", UCRL-MA-130651. Lawrence Livermore National Laboratory, Livermore, CA, 1998.